Report from the CCP13 Working Party on Monday, 3rd August 1992

GRAPHICS

Present: Geoff Mant, Trevor Forsyth, Richard Denny.

The aim of this working party was to identify the criteria for choosing between graphics libraries and to nominate some candidates for incorporation into the CCP13 program suite. The working party considered the following aspects of available packages:

(i)   The chosen package should be both C and FORTRAN callable.
(ii)   The package should drive XII, Postscript and tectronix devices.
(iii)   The package should be portable among a diversity of machines.

Remaining questions are:

(iv)   Should the chosen package be public domain or should users be expected to pay for licences?
(v)   What level of plotting routine is required? For example, is contour plotting essential?

Two packages, Vogle and PGPLOT, were considered in this context.

Vogle is portable, public domain, it drives the appropriate devices and is both C and FORTRAN callable. However, it does not possess any higher level plotting routines. PGPLOT also drives the appropriate devices, has high level plotting routines but it is only (as far as we know) FORTRAN callable.

Opinions on aspects (iv) and (v) and any suggestions for graphics libraries from the fibre diffraction community would be appreciated.

Richard Denny

COVER ILLUSTRATION

High-angle fibre diffraction pattern from a liquid-crystalline gel of racemic poly-γ-benzyl glutamate in the α-helical form produced by swelling a dried oriented fibre in dimethylformamide.   Although the main polypeptide structure is α-helical, the benzyl groups on the long side-chains interact specifically to form a regular structure with a different symmetry to the α-helical backbones.   The strong inner meridional reflection at 10.6Å is from the side-chain structure.   The diffraction pattern was recorded in about 1967 using an Elliott toroid camera on a Hilger microfocus X-ray generator.   It displays many of the key factors involved in analysing fibre diffraction patterns: partial sampling, strong diffuse scattering, arcing of layer-lines. (Squire, J.M., Ph.D Thesis)